THEORY OF MULTIFERROIC MANGANITES – RESEARCH NUGGET Nicola Hill, Materials Department, UC Santa Barbara, DMR-9973076

Multiferroics are materials that are simultaneously ferromagnetic and ferroelectric. Very few exist in nature or have been synthesized in the laboratory, but their potential applications are wide-ranging and could have significant technological impact. Our research has shown that the usual mechanism for ferroelectricity is incompatible with the occurrence of magnetism, and so an alternative driving force for the structural distortion that causes ferroelectricity must be found in order to create a multiferroic material. Figure 1 shows our prediction of such an alternative mechanism - off-center displacement of the Bi cations in BiMnO₃ caused by the stereochemical activity of the Bi lone pairs. Figure 2 shows the ferroelectric hysteresis loops in subsequently synthesized BiMnO₃ which confirm our prediction (from Dos Santos et al., in preparation). This is, to our knowledge, the first prediction of ferroelectricity in a new material, and certainly the first design and subsequent synthesis of a new multiferroic.

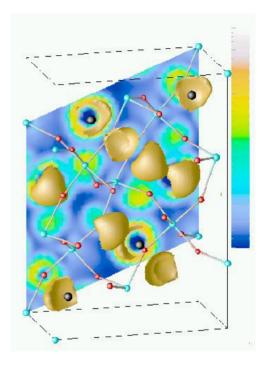
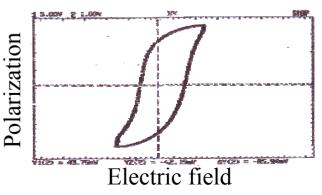


Figure 1. Valence electron localization function of BiMnO₃ calculated in this work. The yellow lobes represent the localized Bi lone pairs which displace the Bi ions and drive ferroelectricity.

Figure 2. Measured ferroelectric hysteresis loops in BiMnO₃ at room temperature.



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In our technologically advanced and globally mobile society, ensuring a scientifically literate work force is a necessity both at home and overseas. During a recent sabbatical spent largely at a major research university in India, I had two unforgettable opportunities to contribute in a small way to international science education and outreach.

It was a tremendous honor for me to be invited to attend the Pakistan Physical Society's annual meeting, where I had the opportunity for extensive technical and social discussions with the undergraduate and graduate students. In particular I was delighted to meet the many intelligent and highly motivated young women who are studying physics in Pakistan, and my presence as a professional female scientist traveling independently generated tremendous excitement among them!





I also participated in an Agilent Technology expedition to install solar-powered refrigerators in rural community medical centers in Nepal. Here I worked with local High School science teachers in the Kanchenjunga Valley, to develop and teach classes on the physics of solar energy technology. The challenges posed by teaching in schools with no walls or water were quite different than those encountered during my regular classroom teaching in California!